ABSTRACT

Disclosed is a method for representing and analyzing 3D target molecule-ligand intermolecular interactions. The method generates structural interaction fingerprints (SIFts) that convert three-dimensional structural interaction information into linear information strings that contains a plurality of information blocks; each of which in turn containing a plurality of information units. By assigning to each information unit a calculated value to represent the characteristic of a set of intermolecular interactions occurring at each selected position (i.e., a position on the target molecule at which intermolecular interaction occurs), a SIFt of the target molecule-ligand complex is constructed.